2,4,5-Trifluorobenzyl alcohol, neopentyl ether

Inchi: InChI=1S/C12H15F3O/c1-12(2,3)7-16-6-8-4-10(14)11(15)5-9(8)13/h4-5H,6-7H2,1-3H3
InchiKey: GAYXXBPRPTYIRS-UHFFFAOYSA-N
Formula: C12H15F3O
SMILES: CC(C)(C)COCc1cc(F)c(F)cc1F
Mol. weight [g/mol]: 232.24

Physical Properties

Property code	Value	Unit	Source
gf	-552.91	kJ/mol	Joback Method
hf	-818.19	kJ/mol	Joback Method
hfus	22.72	kJ/mol	Joback Method
hvap	45.23	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.667		Crippen Method
mcvol	167.360	ml/mol	McGowan Method
pc	2034.55	kPa	Joback Method
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
tb	532.58	K	Joback Method
tc	716.97	K	Joback Method
tf	315.40	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.73	J/mol×K	532.58	Joback Method
cpg	415.04	J/mol×K	563.31	Joback Method
cpg	428.64	J/mol×K	594.04	Joback Method
cpg	441.56	J/mol×K	624.77	Joback Method
cpg	453.82	J/mol×K	655.51	Joback Method
cpg	465.44	J/mol×K	686.24	Joback Method
cpg	476.43	J/mol×K	716.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375251&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume